

Hydrodynamical thermotransport relaxation times of semiconductor electrons via acoustic phonons

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(Dated: February 1, 2008)

We propose a hydrodynamic model to study the thermotransport properties of semiconductor electrons. From the semiclassical Boltzmann equation a set of balance equations is built for the relevant fields. The electron density, the electron energy density, the electric current density and the heat flux density are considered as the basic fields of direct transport and cross effect fluxes. The kinetic relaxation times of the production terms are calculated by considering the electron-acoustic phonon interaction as the leading microscopic scattering process. To justify the long time thermalization regime, the Onsager symmetry relations are proved, both on the completely degenerate and non degenerate limits.

PACS numbers: 05.20.Dd, 72.10.Bg, 72.15.Jf, 72.15.Lh

I. INTRODUCTION

Hydrodynamical models have been widely used to describe thermotransport properties of electrons in semiconductor materials. Complementary contributions of charge transport and thermal dissipation fluxes can be included in the same model, but due to the complexity of the system, and the amount of microscopic processes involved, it is mandatory to separate the analysis of the microscopic scattering processes of electrons.

As usual, a generalized hydrodynamic model of semiconductors requires of constructing a hierarchy of balance equations for the complete set of basic fields from the semiclassical Boltzmann transport equation (BTE)[1]. This hydrodynamic scheme constitutes a closed set of balance equations for the relevant variables once the higher order moments and the production terms have been completely evaluated.

Depending on the order of the approximation, an expansion of the non equilibrium distribution function (NEDF) must be used to calculate the higher order moments by means of the local variables. For example, in degenerate semiconductors, a local Fermi-Dirac distribution function is used as a weight function to take in to account the non equilibrium regime. Most of the complications appear when calculating the production terms corresponding to the non conserved variables. The largest difficulty arises as a result of the intrinsic complexity of the collisional kernel of the BTE, enhanced by the microscopic semiconductor scattering processes of electrons which involve a variety of crystal lattice perturbations.

Due to all these considerations the closure problem is usually solved by including some phenomenological components, such as the relaxation time approximation, or the computational Monte Carlo analysis. The result is a hybrid scheme of thermotransport of electrons between the kinetic and phenomenological models (or ki-

netic and numerical Monte Carlo method)[2, 3]. Following these arguments, we can understand why most of the hydrodynamical models of thermotransport in semiconductors have some approximations in the region of quasi-stationary macroscopic fluxes. In this region, the perturbations drive the system not too far from the local thermodynamic equilibrium, so it is possible to develop a complete kinetic theoretical model considering a specific electron-lattice interaction dominating the thermalization process.

In this work, a kinetic theory approach is considered to solve the semiclassical BTE for the electrons in a semiconductor. The method of moments derives into a set of balance equations up to the 8-fields approximation. The basic fields of the electron density, electric current density, energy density, and heat flux are the local relevant variables. The closure of the balance equations is achieved by using the maximum entropy principle with a NEDF, which allows to evaluate the production terms without any phenomenological assumption, as is commonly done in the literature[1, 4]. The electron-acoustic phonon interaction is the leading scattering mechanism, i.e., the lattice temperature is relatively low. The electric field is absent, however, an internal electric field is generated because of the inhomogeneities of the electron's distribution. The resulting kinetic relaxation times are used to justify the linear hydrodynamic model by checking the corresponding Onsager symmetry relations. This assures that the linear response theory corresponds to the relaxation time approximation.

II. THE KINETIC MODEL

We assume that a macroscopic state of the electrons is characterized by the eight local relevant variables corresponding to the number density of the electron's charge,

$n(\mathbf{x}, t)$, which defines the mass density through $\rho(\mathbf{x}, t) = m n(\mathbf{x}, t)$, where m is the electron's effective mass. The electric current density, $J_i(\mathbf{x}, t) = -en(\mathbf{x}, t) v_i(\mathbf{x}, t)$, where $v_i(\mathbf{x}, t)$ is the hydrodynamic velocity and e is the electrical charge of electrons. The energy density, $W(\mathbf{x}, t)$, is defined as the average of $\mathcal{E} = \frac{1}{2} m C_{\mathbf{k}}^2$. Here, $\mathbf{C}_{\mathbf{k}}$ is the peculiar velocity with components $C_i(\mathbf{x}, \mathbf{k}, t) = c_i(\mathbf{k}) - v_i(\mathbf{x}, t)$ and $c_i(\mathbf{k}) = \hbar k_i / m$ is the velocity of electrons. To complete the set of basic fields, we have denoted by $q_i(\mathbf{x}, t)$ the local heat flux density.

The balance equations for describing the fluxes of electron's charge and energy, according to Refs. [1, 5], are:

$$\begin{aligned} \frac{\partial \rho}{\partial t} - \frac{m}{e} \frac{\partial J_i}{\partial x_i} &= 0, \\ \frac{\partial \rho W}{\partial t} + \frac{\partial q_i}{\partial x_i} - \mathcal{E}_i J_i &= 0, \\ \frac{\partial J_i}{\partial t} - \frac{e K_B}{m^2} \nu T^{\frac{3}{2}} \left(\frac{5}{3} I_4 - \frac{\varphi}{K_B T} I_2 \right) \frac{\partial T}{\partial x_i} \\ &- \frac{e^2}{m^2} \nu T^{\frac{3}{2}} I_2 \mathcal{E}_i = - \left(\frac{J_i}{\tau_J} + \frac{e}{K_B T} \frac{q_i}{\tau_{JQ}} \right), \\ \frac{\partial q_i}{\partial t} + \frac{5 K_B^2}{3 m^2} \nu T^{\frac{5}{2}} \left(\frac{7}{5} I_6 - \frac{\varphi}{K_B T} I_4 \right) \frac{\partial T}{\partial x_i} \\ &+ \frac{5 e K_B}{3 m^2} \nu T^{\frac{5}{2}} I_4 \mathcal{E}_i = - \left(\frac{q_i}{\tau_Q} + \frac{K_B T}{e} \frac{J_i}{\tau_{QJ}} \right). \end{aligned} \quad (1)$$

The effective local electric field is defined by $\mathcal{E}_i = (1/e) \partial \varphi / \partial x_i$, where φ is the local chemical potential. We have defined the constants, $\nu = 2^{9/2} K_B^{3/2} m^{5/2} \pi / \hbar^3$, K_B the Boltzmann constant, \hbar the Planck constant, and denoted by $I_n = I_n(\varphi / K_B T)$ the Fermi-Dirac integrals[4]. Summation over repeated indices has been considered. Note that the production terms, rhs of Eqs. (1), contains contributions to the cross effect fluxes, which are proportional to τ_{JQ}^{-1} and τ_{QJ}^{-1} respectively. They are necessary to compare the constitutive relations of the thermotransport coefficients under a Onsager symmetry criterion.

The closure of the set of generalized hydrodynamic evolution equations is achieved by using a NEDF. This function must be an approximate solution of the Boltzmann equation coming from the maximum entropy principle, which is assumed to be of the form $f = f^{FD}(\mathcal{E})(1 + \Phi)$. The term Φ can be written in terms of the basic fields[1],

$$\Phi = (1 - f_{\mathbf{k}}^{FD}) \left(F_i^{(3)} J_i + G_i^{(3)} q_i \right), \quad (2)$$

where,

$$F_i^{(3)} = \frac{21 m^2}{e \nu K_B T^{\frac{3}{2}}} I_J(\mathcal{E}) C_i(\mathbf{k}), \quad (3)$$

$$G_i^{(3)} = \frac{15 m^2}{\nu K_B^2 T^{\frac{5}{2}}} I_Q(\mathcal{E}) C_i(\mathbf{k}). \quad (4)$$

The functions $I_J(\mathcal{E})$ and $I_Q(\mathcal{E})$ are defined through the Fermi integrals as follows[5],

$$I_J(\mathcal{E}) = \frac{I_6 - \frac{5\mathcal{E}}{7 K_B T} I_4}{25 I_4^2 - 21 I_2 I_6}, \quad (5)$$

and

$$I_Q(\mathcal{E}) = \frac{I_4 - \frac{3\mathcal{E}}{5 K_B T} I_2}{25 I_4^2 - 21 I_2 I_6}. \quad (6)$$

In this semiclassical hydrodynamical model, the weight function $f^{FD}(\mathcal{E})$ is a local Fermi-Dirac distribution function. Also, in Ref. [5] we can see that the relaxation times have the following general form for the electric current density,

$$\begin{aligned} \frac{1}{\tau_J} &= \sum_{\pm} \frac{-em}{3\hbar} \int d\mathbf{k} d\mathbf{k}' S(\mathbf{k}, \mathbf{k}') (\mathbf{k}' - \mathbf{k}) \\ &\left[f_{\mathbf{k}}^{FD} (1 - f_{\mathbf{k}}^{FD}) (1 - f_{\mathbf{k}'}^{FD}) F_i^{(3)} \right. \\ &\quad \left. - f_{\mathbf{k}}^{FD} f_{\mathbf{k}'}^{FD} (1 - f_{\mathbf{k}'}^{FD}) F_i^{(3)'} \right], \end{aligned} \quad (7)$$

and for the heat flux density,

$$\begin{aligned} \frac{1}{\tau_Q} &= \sum_{\pm} \frac{m^2}{6\hbar} \int d\mathbf{k} d\mathbf{k}' S(\mathbf{k}, \mathbf{k}') (\mathcal{E}' \mathbf{k}' - \mathcal{E} \mathbf{k}) \\ &\left[f_{\mathbf{k}}^{FD} (1 - f_{\mathbf{k}}^{FD}) (1 - f_{\mathbf{k}'}^{FD}) G_i^{(3)} \right. \\ &\quad \left. - f_{\mathbf{k}}^{FD} f_{\mathbf{k}'}^{FD} (1 - f_{\mathbf{k}'}^{FD}) G_i^{(3)'} \right]. \end{aligned} \quad (8)$$

Similar expressions have been found for the cross effect fluxes. The signs under the summation symbol indicate absorption and emission respectively.

III. THE RELAXATION TIMES

To evaluate the kinetic relaxation times, we must specify an electron-phonon interaction according to the perturbations in the crystal lattice. In the present case, we have considered interactions with acoustic phonons as the leading mechanism of the collisional processes of electrons. As usual, the rate of electron collisions with acoustic phonons is given by[8],

$$S(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \left[\frac{D_{ac}^2 K_B T}{2 L^3 \rho v_s^2} \right] \delta(\mathcal{E} - \mathcal{E}') \quad (9)$$

where D_{ac} is the electron-acoustic phonons deformation potential, and v_s represents the velocity of sound. After a substitution of Eq. (9) into Eqs. (7-8) and considering that the electron energy \mathcal{E} is the integration variable, we obtain general expressions for the relaxation times.

The corresponding relaxation time for the electric current density is,

$$\tau_J^{-1} = \frac{7}{2} \frac{(2\pi)^2 D_{ac}^2 m^{\frac{3}{2}}}{\hbar^4 \rho v_s^2 (K_B T)^{\frac{1}{2}}} \int I_J(\mathcal{E}) [f^{FD}(\mathcal{E})]^2 (1 - f^{FD}(\mathcal{E})) \mathcal{E}^2 d\mathcal{E} \quad (10)$$

A similar procedure gives rise to all the other relaxation time expressions. The following are the expressions for $1/\tau_Q$, $1/\tau_{JQ}$, and $1/\tau_{QJ}$. For the heat flux we have,

$$\tau_Q^{-1} = \frac{5}{2} \frac{(2\pi)^2 D_{ac}^2 m^{\frac{3}{2}}}{\hbar^4 \rho v_s^2 (K_B T)^{\frac{3}{2}}} \int I_Q(\mathcal{E}) [f^{FD}(\mathcal{E})]^2 (1 - f^{FD}(\mathcal{E})) \mathcal{E}^3 d\mathcal{E} \quad (11)$$

and the crossed effect relaxation times, τ_{JQ} and τ_{QJ} , are given by,

$$\tau_{JQ}^{-1} = \frac{5}{2} \frac{(2\pi)^2 D_{ac}^2 m^{\frac{3}{2}}}{\hbar^4 \rho v_s^2 (K_B T)^{\frac{1}{2}}} \int I_Q(\mathcal{E}) [f^{FD}(\mathcal{E})]^2 (1 - f^{FD}(\mathcal{E})) \mathcal{E}^2 d\mathcal{E} \quad (12)$$

$$\tau_{QJ}^{-1} = \frac{7}{2} \frac{(2\pi)^2 D_{ac}^2 m^{\frac{3}{2}}}{\hbar^4 \rho v_s^2 (K_B T)^{\frac{3}{2}}} \int I_J(\mathcal{E}) [f^{FD}(\mathcal{E})]^2 (1 - f^{FD}(\mathcal{E})) \mathcal{E}^3 d\mathcal{E}. \quad (13)$$

By incorporating this expressions of the relaxation times in the hydrodynamical set of transport equations we obtain a completely closed model containing no free or phenomenological parameters. It is very important to note that though the structure of the transport equations is given, and does not depend on a microscopic model for the interaction, the specific values of the relaxation times depend closely on the model of the electron-lattice interaction.

IV. ONSAGER SYMMETRY

As is well known, the Onsager symmetry principle projects microscopic reversibility of the interactions onto a macroscopic scale through the transport symmetry relations. In this section we will show that, in the linear response regime, the semiconductor transport of charge, under internal electric fields variations and thermal gradients, can be characterized by a set of constitutive relations with thermoelectric transport coefficients displaying symmetry on the cross effect fluxes. This point deserves some discussion because the microscopic interactions of the semiconductor electrons are regulated by a process of creation and annihilation of phonons. So there

is no guarantee of microscopic reversibility. However, because of the elastic collision between electrons and acoustic phonons, our result reflects the existence of a kind of a more general detailed balance principle of collisions.

We show the validity of the Onsager symmetry relations, at the end of the thermalization process and both in the completely degenerate as well non degenerate limits, by following a general expression that must be satisfied (see Ref. [1]):

$$\tau_J \left(5I_4 - 3I_2 \frac{\tau_Q}{\tau_{QJ}} \right) = -\tau_Q \left(5I_4 - 7I_6 \frac{\tau_J}{\tau_{JQ}} \right). \quad (14)$$

First, we are considering the kinetic relaxation times in the complete degenerate limit. In this case, integration with respect to energy, and assuming the Fermi-Dirac distribution function satisfying $f^{FD}(\mathcal{E}) (1 - f^{FD}(\mathcal{E})) = \delta(\mathcal{E} - \varphi)$, derives into the following expressions for the relaxation times:

$$\begin{aligned} \tau_J^{-1} &= \frac{7}{2} v \frac{I_6 - \frac{5\varphi}{7K_B T} I_4}{25I_4^2 - 21I_2 I_6}, \\ \tau_Q^{-1} &= \frac{5}{2} v \frac{I_4 - \frac{3\varphi}{5K_B T} I_2}{25I_4^2 - 21I_2 I_6} \frac{\varphi}{K_B T}, \\ \tau_{JQ}^{-1} &= \frac{5}{2} v \frac{I_4 - \frac{3\varphi}{5K_B T} I_2}{25I_4^2 - 21I_2 I_6}, \\ \tau_{QJ}^{-1} &= \frac{7}{2} v \frac{I_6 - \frac{5\varphi}{7K_B T} I_4}{25I_4^2 - 21I_2 I_6} \frac{\varphi}{K_B T}. \end{aligned} \quad (15)$$

Here, we have introduced the parameter v , which depends on the chemical potential of electrons and the local temperature,

$$v = \left(\frac{2\pi m D_{ac} \varphi}{K_B T} \right)^2 \sqrt{\frac{K_B T}{m}} \frac{K_B T}{\hbar^4 \rho v_s^2}. \quad (16)$$

A direct substitution of these expressions into the Onsager conditions show us that they are well satisfied. On the non degenerate case, the Onsager symmetry relation is well satisfied too. If we consider this limit, $f^{FD}(\mathcal{E}) \ll 1$ and it becomes a Maxwellian distribution function. Under these conditions the relaxation times can be expressed as follows,

$$\begin{aligned} \tau_J^{-1} &= \frac{1}{4} \nu_1 \left(\frac{K_B T}{2} \right)^3 \frac{2! (14I_6 - 15I_4)}{(25I_4^2 - 21I_2 I_6)} \\ \tau_Q^{-1} &= \frac{1}{2} \nu_3 \left(\frac{K_B T}{2} \right)^4 \frac{3! (5I_4 - 6I_2)}{(25I_4^2 - 21I_2 I_6)} \\ \tau_{JQ}^{-1} &= \frac{1}{2} \nu_1 \left(\frac{K_B T}{2} \right)^3 \frac{1! (10I_4 - 9I_2)}{(25I_4^2 - 21I_2 I_6)} \\ \tau_{QJ}^{-1} &= \frac{1}{2} \nu_3 \left(\frac{K_B T}{2} \right)^4 \frac{3! (7I_6 - 10I_4)}{(25I_4^2 - 21I_2 I_6)} \end{aligned} \quad (17)$$

here we have defined the parameters,

$$\nu_n = \frac{(2\pi D_{ac})^2 m^{\frac{3}{2}}}{\hbar^4 \rho v_s^2 (K_B T)^{\frac{n}{2}}} \exp \left(\frac{2\varphi}{K_B T} \right), \quad n = 1, 2, \dots \quad (18)$$

Once again, the Onsager condition is well satisfied in this case. Next, what we can see is if the full integral expressions for the kinetic relaxation times satisfy the symmetry condition. However, this requires a computational analysis and a correct interpretation of the numerical uncertainties. We can speculate that the Onsager symmetry is going to be well satisfied in all the interval of the temperature variations, because of the regime in which we are working (the last stage of thermalization) and the assumption of the microscopic detailed balance under elastic electron-phonon collision being satisfied.

The general condition of symmetry, in Eq. (14), also appears in Refs. [1, 5], among others, with respect to the Onsager symmetry relations of the thermotransport coefficients. In particular in Ref. [5] it is shown that for thermotransport in polar semiconductors, where the main microscopic interaction mechanism is the electron-polar optical phonons, the relation specifies that only some values of φ are satisfying the symmetry condition, i.e., only certain values are allowed for the chemical potential in comparison to the optical phonon energy. Though this condition seems a very restrictive one, we must note that the model corresponds only to the behavior of electron population. The phonons become the reservoir of lattice perturbations, so they are not taken into account in order to preserve microscopic reversibility[7]. Hence the Onsager symmetry relation depends strongly on the thermalization regime where a different microscopic electron-lattice interactions may be dominating the relaxation processes.

V. DISCUSSION AND CONCLUSIONS

We have developed a kinetic theoretical approach to describe a generalized hydrodynamic behavior of semiconductor electrons at the end of the thermalization process. The semiclassical Boltzmann transport equation have been solved up to the eight moments method approximation in such a way that the heat flux density is considered as a relevant variable in the resulting hydrodynamical model. The closure of the balance equations is achieved by evaluating the higher order moments, as well as the production terms, through a non equilibrium distribution function according to the maximum entropy principle as has been described in literature. In case that the electron-acoustic phonon scattering is the leading mi-

croscopic interaction, the production terms can be expressed by means of a set of kinetic relaxation times.

As a consequence of the theoretical model developed in this paper, we have shown analytically that condition (14) is satisfied in both degenerate and non degenerate limits. This means that Onsager symmetry relations are fulfilled. Even more, and given that for the electron-acoustic phonon scattering the microscopic reversibility is valid, we believe that the general expressions for the relaxation times, Eqs. (10)–(13), will give that Onsager symmetry relations are also satisfied under more general conditions.

In general, the electron transport properties in semiconductors depend on the scattering processes that electrons suffer. In addition, these transport processes can be expressed in terms of the relaxation times for each scattering mechanism. Relaxation times are usually obtained by Monte Carlo Simulations[9]. For the case of electron-acoustic phonon interaction we have found closed general expressions, Eqs. (10)–(13), which together with the general expressions found in Ref. [5] for electron-optical phonon interaction provide us with a theoretical framework to describe the thermotransport processes of electrons in semiconductors under more general conditions with no free or phenomenological parameters. A complete scheme will be obtained when we include electron-intervalley phonons and electron-impurity scattering processes. The case of piezoelectric phonon perturbations is rather direct and follows the same argument as acoustic phonon perturbations. A detailed analysis of the relaxation times as function of lattice temperature and electron concentration will give us useful information of the main relaxation channel under the imposed conditions[7, 10]. For example, in Ref. [9] it is shown that, for a silicon device, the energy relaxation time (which is the characteristic time in which the electron energy relaxes to the lattice) is substantially larger than the relaxation times for momentum and heat flux. The situation could be very different for Bulk GaAs. For high temperatures (300 K) and low electron concentration (of the order or less than 10^{16} cm^{-3}) the main collision mechanism is electron-acoustic interactions. Whereas, for low temperatures and high electron concentration where screening effect should be taken into account, the electron-optical phonon interaction should be the main relaxation mechanism[7].

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